Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electroninc Supplementary Information (ESI)

Solvent Sensitive Intramolecular Charge Transfer Dynamics in the Excited States of 4-N,N-Dimethylamino-4'-nitrobiphenyl

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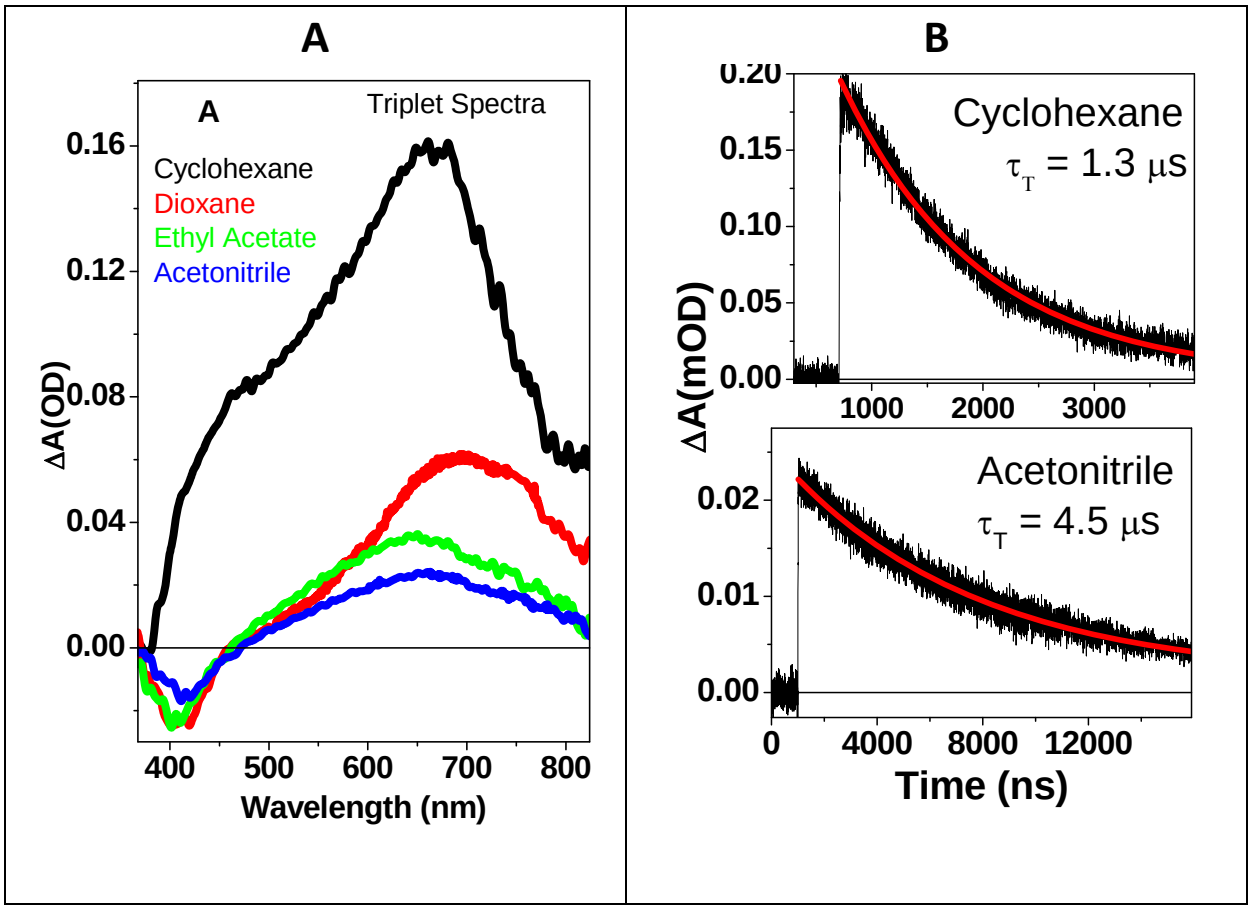

Fig. S1: (A) Transient absorption spectra of DNBP in different solvents (in argon atmosphere) recording at 10 nanosecond delay time following photoexcitation using 355 nm laser pulses. Sample absorption at 355 nm (OD = 0.3) and excitation pulse energy (10mJ/pulse) were kept same for all solvents. (B) Triplet lifetime in cyclohexane and acetonitrile.

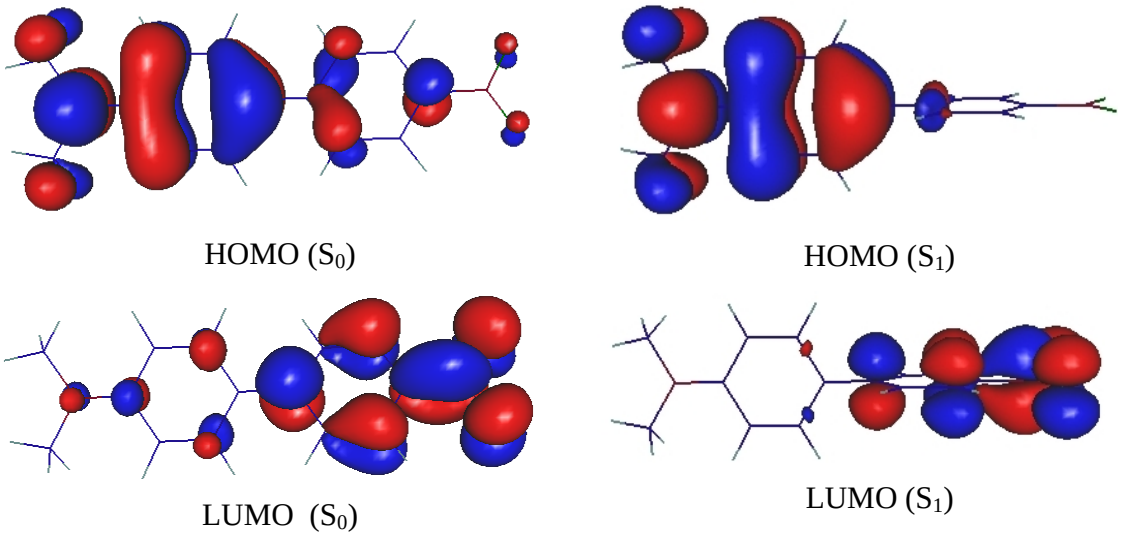

Fig. S2: HOMO and LUMO orbital compositions in the ground electronic state (S_0) (left) and the first excited state (S_1) (right) with the optimized geometries.

Table T1: Lifetimes and the corresponding amplitudes associated with the multiexponential functions to best fit the temporal profiles recorded at different wavelengths following photoexcitation of DNBP in acetonitrile (IRF ~120 fs).

Probe wavelength	Lifetimes (amplitude)
540 nm	IRF (-0.2) 0.48 ps (+1.0) 3.0 ps (-0.7)
750 nm	IRF (+0.28) 0.3 ps (-1.0) 2.7 ps (+0.72)
810 nm	IRF (+0.22) 0.35 ps (-1.00) 2.8 ps (+0.78)
900 nm	IRF (-0.05) 0.45 ps (-0.95) 2.9 ps (+1.0)

Table T2: Lifetimes and the corresponding amplitudes associated with the multiexponential functions to best fit the temporal profiles recorded at 630 and 860 nm following photoexcitation of DNBP in ethyl acetate (IRF ~120 fs).

Probe wavelength	Lifetimes (amplitude)
630 nm	IRF (-0.7) 0.48 ps (-0.3) 4.4 ps (0.35) 66 ps (0.65)
860 nm	IRF (+0.6) 4.2 ps (-1.0) 70 ps (+0.4)

Table T3: Lifetimes and the corresponding amplitudes associated with the multiexponential functions to best fit the temporal profiles recorded at 530, 630 and 690 nm following photoexcitation of DNBP in 1, 4-dioxane (IRF ~120 fs).

Probe wavelength	Lifetimes (amplitude)
500 nm	IRF (-1.0) 2.4 ps (+0.70) 30 ps (+0.30)
630 nm	IRF (+0.1) 3.1 ps (-0.9) 35 ps (-0.1) Long ns (+0.9)
690 nm	IRF (+0.15) 3.0 ps (-0.6) 30 ps (-0.4) Long ns (+0.85)

Table T4: Lifetimes and the corresponding amplitudes associated with the multiexponential functions to best fit the temporal profiles recorded at 480 and 670 nm following photoexcitation of DNBP in cyclohexane (IRF ~120 fs).

Probe wavelength	Lifetimes (amplitude)
480 nm	IRF (+1.0) 0.8 ps (-0.5) 10.2ps (-0.3) Long ns (-0.2)
670 nm	IRF (+0.05) 4.2 ps (+0.95) Long ns (-1.0)